

PHOTON OPACITY IN SURFACES OF MAGNETIC NEUTRON STARS

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ABSTRACT

Approximate expressions are derived for free-free, bound-free, and Thomson cross-sections of photons by gaseous matter in the presence of superstrong magnetic fields. For photons in modes whose electric field polarization is perpendicular to this magnetic field, the cross-section is reduced by approximately the squared ratio of the photon frequency to the electron cyclotron frequency if this ratio is small.

Subject headings: neutron stars — opacities — plasmas — polarization

I. INTRODUCTION

The huge magnetic fields which thread neutron stars dominate the motion of electrons in the stellar surfaces. In estimated surface fields $H \sim 10^{12}$ – 10^{13} gauss, $\hbar\omega_H \equiv ehH/m_e c = 10^4$ – 10^5 eV. This is much greater than the estimated thermal energies of surface electrons and X-rays in all known pulsars. In the presence of such strong fields, the cross-sections for the Thomson, free-free, and bound-free transitions are greatly reduced over the field-free values if the electric field vector \mathbf{E} of the incident electromagnetic wave is perpendicular to \mathbf{H} . This is because a sufficiently strong magnetic field tends to confine the motion of electrons to that of \mathbf{H} and suppresses their response to any perpendicular force.

There are two independent modes for an electromagnetic wave in a magnetized plasma, viz., the ordinary (O) mode and the extraordinary (X) mode. A detailed examination of the polarization of these two modes shows that if $\omega \ll \omega_H$ and $\omega \gtrsim$ the plasma frequency $(4\pi n_e e^2/m_e)^{1/2}$, then the \mathbf{E} vector of the X-mode will essentially always be perpendicular to \mathbf{H} , and the \mathbf{E} vector of the O-mode will be perpendicular to \mathbf{H} for propagation along \mathbf{H} but becomes parallel to \mathbf{H} for other directions of propagation (Canuto, Lodenquai, and Ruderman 1971). Therefore, the X-mode photons generally have a much longer mean free path than O-mode photons and give the main contribution to radiation transport in a neutron star surface.

When $\omega \ll \omega_H$, the mean squared amplitude response of a free electron to an oscillating electric field perpendicular to \mathbf{H} is reduced by $(\omega/\omega_H)^2$ from that when $H = 0$. This factor was used by us (Tsuruta *et al.* 1972) to estimate the opacity and cooling rates of magnetized neutron stars. In the present paper we justify, for photons with \mathbf{E} perpendicular to \mathbf{H} , the approximate relation between cross-sections with and without superstrong magnetic fields:

$$\sigma_{\perp}(H) \simeq (\omega/\omega_H)^2 \sigma(0); \quad \omega \ll \omega_H. \quad (1)$$

The relationship of equation (1) holds for all the major processes contributing to photon opacity. In § II, we review briefly the properties of an electron in a magnetic field. In §§ III, IV, and V we treat the Thomson, free-free, and bound-free transitions, respectively, in superstrong magnetic fields ($H \gtrsim 10^{12}$ gauss). In § VI we examine the effects of the bound-bound transition on the radiative opacity.

In this paper and the previous one (Tsuruta *et al.* 1972) we neglect the contribution of electrons to energy transport at the stellar surface. This mode of transport is unimportant in the nondegenerate surface layers of conventional stars. But magnetized neutron stars can have energetic degenerate electrons extending right to the edge of the star (Ruderman 1971, 1972). These would contribute to energy transport and increase our previously estimated cooling rates.

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II. ELECTRON IN A MAGNETIC FIELD

The Schrödinger equation for an electron in a uniform, static magnetic field \mathbf{H} is

$$-\frac{\hbar^2}{2m_e} \left[\frac{1}{\rho} \frac{\partial}{\partial \rho} \left(\rho \frac{\partial \psi}{\partial \rho} \right) + \frac{\partial^2 \psi}{\partial z^2} + \frac{1}{\rho^2} \frac{\partial^2 \psi}{\partial \phi^2} \right] - \frac{i\hbar\omega_H}{2} \frac{\partial \psi}{\partial \phi} + \frac{1}{8} m_e \omega_H^2 \rho^2 \psi - \boldsymbol{\mu} \cdot \mathbf{H} \psi = E \psi \quad (2)$$

in cylindrical polar coordinates (ρ, ϕ, z) . The magnetic field is assumed to be along the z -direction. The vector potential is chosen to have components

$$A_\phi = \frac{1}{2} H \rho, \quad A_z = A_\rho = 0; \quad (3)$$

$\boldsymbol{\mu}$ is the Dirac magnetic moment of the electron. The solution of equation (2) (neglecting the spin wave function, which is separable) is (Landau and Lifshitz 1965)

$$\psi_{n_\rho, m, k} = \frac{e^{ikz}}{L^{1/2}} \frac{e^{im\phi}}{(2\pi)^{1/2}} C_{n_\rho, m}(2\gamma)^{1/2} e^{-\xi/2} \xi^{|m|/2} F(-n_\rho, |m| + 1, \xi) \equiv |n_\rho, m, k\rangle, \quad (4)$$

where L is the normalization length along \mathbf{H} . The parameter $\xi \equiv (eH/2\hbar c)\rho^2 \equiv \gamma\rho^2$; $F(-n_\rho, |m| + 1, \xi)$ is the confluent hypergeometric function; $m (=0, \pm 1, \pm 2, \dots)$ is the angular-momentum quantum number; n_ρ is a positive integer or zero. $C_{n_\rho, m}$ is a normalization constant given by

$$|C_{n_\rho, m}|^2 = \frac{(|m| + 1)(|m| + 2) \cdots (|m| + n_\rho)}{|m|! n_\rho!} \quad \text{for } n_\rho \neq 0, \\ |C_{0, m}|^2 = \frac{1}{|m|!} \quad \text{for } n_\rho = 0. \quad (5)$$

The energy eigenvalues of equation (2) are

$$E_{n_\rho, m, k, \sigma} = \hbar\omega_H \left(n_\rho + \frac{\sigma}{2} + \frac{|m|}{2} + \frac{m}{2} + \frac{1}{2} \right) + \frac{p_z^2}{2m_e}, \quad (6)$$

with $\sigma = \pm 1$ corresponding to electron spin parallel or antiparallel to the magnetic field; $p_z \equiv \hbar k$ is the electron momentum along z , i.e., along the magnetic field. If m is negative or zero, the eigenvalues reduce to

$$E_{n_\rho, -|m|, k, \sigma} = (n_\rho + \frac{1}{2}\sigma + \frac{1}{2})\hbar\omega_H + p_z^2/2m_e, \quad (7)$$

which is independent of m : all the states of zero and negative m are degenerate. The lowest energy state corresponds to $n_\rho = 0$, $\sigma = -1$ in equation (7), i.e.,

$$E_{0, -|m|, k, -1} = p_z^2/2m_e. \quad (8)$$

In this case, the eigenfunction becomes

$$\psi_{0, -|m|, k} = \frac{e^{ikz}}{L^{1/2}} \frac{e^{-i|m|\phi}}{(2\pi)^{1/2}} (2\gamma)^{1/2} C_{0, -|m|} e^{-\xi/2} \xi^{|m|/2} \equiv |0, -|m|, k\rangle. \quad (9)$$

The first excited state has an energy $\hbar\omega_H$ above the ground state. This corresponds to $n_\rho = 1$ or $m = 1$ or $\sigma = 1$. If $H \sim 10^{12}$ gauss, then $\hbar\omega_H \sim 12$ keV, which is much greater than the typical value of kT in the neutron-star magnetosphere during radiative cooling. In the following, we shall assume therefore that the electrons always have $n_\rho = 0$, $m = 0$ or a negative integer, and $\sigma = -1$, i.e., spin antiparallel to \mathbf{H} .

The electrons have a cylindrically symmetric probability distribution when $n_\rho = 0$; its average radius for a given angular momentum quantum number m is given by

$$\rho_m = (2|m| + 1)^{1/2} \rho_0, \quad (10)$$

where $\rho_0 = (\hbar c/eH)^{1/2}$ is the minimum quantum-mechanical zero-point vibration amplitude transverse to \mathbf{H} .

III. THOMSON SCATTERING

Thomson scattering in a magnetized plasma was treated in detail in a previous paper (Canuto *et al.* 1971). The scattering cross-sections for the two modes of propagation were studied separately. If θ is the angle between \mathbf{H} and the wave vector of the incident electromagnetic wave, we have, for $\theta \rightarrow 0$,

$$\sigma_o(\theta; H) \simeq \sigma_{\text{Th}} \left[\frac{\omega^2}{(\omega_H + \omega)^2} + \frac{1}{2} \sin^2 \theta \right], \quad \sigma_x(\theta; H) \simeq \sigma_{\text{Th}} \left[\frac{\omega^2}{(\omega_H - \omega)^2} + \frac{1}{2} \sin^2 \theta \right]. \quad (11)$$

For $\theta \rightarrow \pi/2$,

$$\sigma_o(\theta; H) \simeq \sigma_{\text{Th}} \sin^2 \theta, \quad \sigma_x(\theta; H) \simeq \sigma_{\text{Th}} \left[\frac{\omega^2}{(\omega_H - \omega)^2} + \cos^2 \theta \right]. \quad (12)$$

In the above $\sigma_{\text{Th}} \equiv (8\pi/3)(e^2/m_e c^2)^2$ is the field-free Thomson cross-section. Equations (11) and (12) are valid if $\omega_p/\omega \ll 1$, where ω_p is the plasma frequency. We then have, for the X-mode,

$$\sigma_x(H)/\sigma(0) \approx (\omega/\omega_H)^2 \quad \text{for } \omega_H \gg \omega, \quad (13)$$

a reasonable approximation for all θ .

IV. FREE-FREE ABSORPTION

The total Hamiltonian of the system in this case can be conveniently regrouped as

$$\hat{H} = \hat{H}_H - \frac{Z'e^2}{(z^2 + \rho_{\bar{m}}^2)^{1/2}} - Z'e^2 \left[\frac{1}{(z^2 + \rho^2)^{1/2}} - \frac{1}{(z^2 + \rho_{\bar{m}}^2)^{1/2}} \right] + \hat{H}_{\text{int}} \quad (14)$$

when the electron is under the influence of the magnetic field and also of the Coulomb field of an ion with charge $Z'e$. \hat{H}_H is the Hamiltonian of an electron in the magnetic field alone as given in equation (2). We define $\rho_{\bar{m}}$ by

$$\rho_{\bar{m}} = (2\bar{m} + 1)^{1/2} \rho_0 \quad (15)$$

where \bar{m} is an arbitrary constant. \hat{H}_{int} is the interaction Hamiltonian. For absorption or emission of a photon, by an electron:

$$\hat{H}_{\text{int}} = \frac{eA_0 \hat{\pi} \cdot \epsilon}{m_e c} e^{\mp i\omega t}, \quad (16a)$$

where $A_0 \equiv c(2\pi\hbar/\omega V_\gamma)^{1/2}$ and V_γ is a normalization volume for photons; $\hat{\pi} \equiv (\hat{p} - eA/c)$ is the canonical momentum of the electron in the magnetic field; ϵ is the polarization unit vector of the photon. An equivalent form for matrix elements between eigenstates of equations (4) and (6) and $\hbar\omega_{\alpha\beta} = E_\alpha - E_\beta$ is

$$\hat{H}_{\text{int}} = -eE(t) \cdot \mathbf{r}, \quad (16b)$$

where $E(t)$ is the electric field vector of the photon. In the case of the X-mode where $E \perp H$, we have $\hat{H}_{\text{int}} = -eE(t)_\rho \cos \phi$. Since $cE(t) = -\partial A(t)/\partial t = -i\omega A(t)$, where $A(t)$ is the vector potential of the photon field, we have for $E \perp H$ the equivalent form

$$\hat{H}_{\text{int}} = \frac{i\omega e A_0}{c} \rho \cos \phi e^{\mp i\omega t}. \quad (17)$$

To the lowest order, the matrix element for free-free transition in this case is

$$M_{\perp}^{\text{ff}} = \frac{i\omega e A_0}{c} \sum_{n_\rho, k''} \left\{ \frac{\langle 0, -|m| + 1, k' | \rho \cos \phi | n_\rho, -|m|, k'' \rangle \langle n_\rho, -|m|, k'' | (V_{\bar{m}} - V_\rho) - V_{\bar{m}} | 0, -|m|, k \rangle}{n_\rho \hbar \omega_H + \hbar \omega} \right. \\ \left. + \frac{\langle 0, -|m| + 1, k' | (V_{\bar{m}} - V_\rho) - V_{\bar{m}} | n_\rho, -|m| + 1, k'' \rangle \langle n_\rho, -|m| + 1, k'' | \rho \cos \phi | 0, -|m|, k \rangle}{n_\rho \hbar \omega_H - \hbar \omega} \right\}. \quad (18)$$

The unperturbed states $|n_\rho, m, k\rangle$ are the eigenfunctions of \hat{H}_H of equation (4), and

$$V_\rho \equiv \frac{Z'e^2}{(z^2 + \rho^2)^{1/2}}; \quad V_{\bar{m}} \equiv \frac{Z'e^2}{(z^2 + \rho_{\bar{m}}^2)^{1/2}}. \quad (19)$$

Since we have assumed $(\omega/\omega_H) \ll 1$, and ω_H appears in the denominator of M_{\perp}^{ff} as $n_\rho \hbar \omega_H$, the leading term in the summation over n_ρ is the first term, with $n_\rho = 0$. It is shown in Appendix A that

$$\langle 0, -|m| + 1, k'' | \rho \cos \phi | n_\rho, -|m|, k'' \rangle = \delta_{k'k''} \delta_{n_\rho, 0} (|m|/\gamma)^{1/2}, \quad (20a)$$

$$\langle n_\rho, -|m| + 1, k'' | \rho \cos \phi | 0, -m, k \rangle = \delta_{kk''} \left(\frac{C_{n_\rho, -|m|+1} C_{0, -|m|}}{\gamma} \right)^{1/2} J_{-n_\rho, |m|}^{|m|}, \quad (20b)$$

where

$$\begin{aligned} J_{-n_\rho, |m|}^{|m|} &= |m|! && \text{for } n_\rho = 0, \\ &= -(|m| - 1)! && \text{for } n_\rho = 1, \\ &= 0 && \text{otherwise,} \end{aligned} \quad (21)$$

$\gamma = eH/2\hbar c$, and $C_{n_\rho, m}$ are the normalization constants given in equation (5). We have then for M_{\perp}^{tr}

$$\begin{aligned} M_{\perp}^{\text{tr}} \simeq \frac{ieA_0}{\hbar c} \left(\frac{|m|}{\gamma} \right)^{1/2} [\langle 0, -|m|, k' | (V_{\bar{m}} - V_\rho) - V_{\bar{m}} | 0, -|m|, k \rangle \\ - \langle 0, -|m| + 1, k' | (V_{\bar{m}} - V_\rho) - V_{\bar{m}} | 0, -|m| + 1, k \rangle]. \end{aligned} \quad (22)$$

Since \bar{m} was introduced as an arbitrary constant, we can choose it for convenience such that

$$\langle 0, -|m|, k' | V_\rho | 0, -|m|, k \rangle \equiv \langle 0, -|m|, k' | V_{\bar{m}} | 0, -|m|, k \rangle = \langle k' | V_{\bar{m}} | k \rangle. \quad (23)$$

The last step follows because $V_{\bar{m}}$ depends only upon z . Then from equation (23)

$$\langle 0, -|m| + 1, k' | V_\rho | 0, -|m| + 1, k \rangle \equiv \langle 0, -|m| + 1, k' | V_{\bar{m} + \delta\bar{m}} | 0, -|m| + 1, k \rangle = \langle k' | V_{\bar{m} + \delta\bar{m}} | k \rangle$$

with $\delta\bar{m} \sim 1$. (24)

Therefore,

$$M_{\perp}^{\text{tr}} \sim \frac{ieA_0}{\hbar c} \left(\frac{|m|}{\gamma} \right)^{1/2} [\langle k' | V_{\bar{m} + \delta\bar{m}} | k \rangle - \langle k' | V_{\bar{m}} | k \rangle] \simeq \frac{ieA_0}{\hbar c} \left(\frac{|m|}{\gamma} \right)^{1/2} \frac{\partial}{\partial \bar{m}} \langle k' | V_{\bar{m}} | k \rangle. \quad (25)$$

The integral in the matrix element,

$$\langle k' | V_{\bar{m}} | k \rangle \equiv \frac{Z' e^2}{L} \int_{-\infty}^{\infty} \frac{e^{i(k' - k)z}}{(z^2 + \rho_{\bar{m}}^2)^{1/2}} dz, \quad (26)$$

is just a Fourier-Bessel transform (Ryshik and Gradstein 1963):

$$\int_{-\infty}^{\infty} \frac{e^{i\Delta kz}}{(z^2 + \rho_{\bar{m}}^2)^{1/2}} dz = 2K_0(\rho_{\bar{m}}\Delta k), \quad (27)$$

where $K_0(x)$ is the modified Hankel function of zero index. We consider below only the two limiting cases of this integral: (a) $\rho_0\Delta k \gg 1$ and therefore $\rho_{\bar{m}}\Delta k \equiv (2\bar{m} + 1)^{1/2}\rho_0\Delta k \gg 1$, the limit of infinite momentum transfer. In this case

$$K_0(\rho_{\bar{m}}\Delta k) \xrightarrow{\rho_0\Delta k \gg 1} \left(\frac{\pi}{2\rho_{\bar{m}}\Delta k} \right)^{1/2} \exp(-\rho_{\bar{m}}\Delta k). \quad (28)$$

(b) $\rho_0\Delta k \ll 1$. In this case there exist two possibilities: (i) there is a range of values of \bar{m} for which $\rho_{\bar{m}}\Delta k \ll 1$ and (ii) a range of values for which $\rho_{\bar{m}}\Delta k \gg 1$. When $\rho_0\Delta k \ll 1$ and $\rho_{\bar{m}}\Delta k \ll 1$ also,

$$K_0(\rho_{\bar{m}}\Delta k) \xrightarrow{\rho_{\bar{m}}\Delta k \ll 1} -\left[\ln \frac{\rho_{\bar{m}}\Delta k}{2} + 0.577 \right]. \quad (29)$$

But for increasing values of m (and therefore \bar{m}), a value of \bar{m} is reached such that $\rho_{\bar{m}}\Delta k \sim 1$ and above which $\rho_{\bar{m}}\Delta k > 1$, achieving finally the asymptotic regime $\rho_{\bar{m}}\Delta k \gg 1$ given by equation (28).

To calculate the cross-section we need the transition probability per unit time:

$$W = \frac{2\pi}{\hbar} |M_{\perp}^{\text{tr}}|^2 \rho(E_f), \quad (30)$$

where $\rho(E_f)$ is the density of final states per unit energy at E_f in a superstrong magnetic field at fixed m and n_ρ :

$$\rho(p_z) = \frac{m_e L}{\pi \hbar p_z}, \quad (31)$$

where L is the plane-wave normalization length and p_z the final momentum along z . For the regime $\rho_0 \Delta k \gg 1$, we have from equations (25)–(28)

$$M_{\perp}^{\text{ff}} \xrightarrow{\rho_0 \Delta k \gg 1} -\frac{ieA_0 Z' e^2}{\hbar c L} \left(\frac{\pi \rho_0 \Delta k}{2^{1/2} \gamma \bar{m}^{1/2}} \right)^{1/2} \exp[-(2\bar{m})^{1/2} \rho_0 \Delta k], \quad (32)$$

The transition rate then is

$$W = \frac{4\pi^2 Z'^2 \alpha_f^3 c^3 m_e (\rho_0 \Delta k) \exp[-2(2\bar{m})^{1/2} \rho_0 \Delta k]}{2^{1/2} V_\gamma L \gamma p_z \omega |m|^{1/2}}, \quad (33)$$

where $\alpha_f \equiv e^2/\hbar c$ is the fine-structure constant and V_γ is the photon normalization volume. The cross-section for photon absorption by an electron in a given m state is found by dividing W by the flux of incident photons $F = c/V_\gamma$ and multiplying by $N(m)$, the total number of electrons in the m th state:

$$N(m)dm = NP(m)dm, \quad (34)$$

where N is the total number of electrons and $P(m)dm$ is the probability that the electron has angular momentum between m and $m + dm$. Because of the symmetry of the wave functions it is convenient to choose the electron normalization volume to be a cylinder of length L and radius R . Then

$$P(m)dm = \frac{2\pi \rho_m d\rho_m}{\pi R^2} \xrightarrow{m \gg 1} \frac{\pi dm}{\gamma(\pi R^2)}. \quad (35)$$

From equations (33)–(35) we obtain the partial cross-section from the state m :

$$\sigma_{\perp}^{\text{ff}}(m) \simeq \frac{2^{7/2} Z'^2 \pi^3 \alpha_f^3 c^2 \hbar \Delta k n_e \exp[-2(2|m|)^{1/2} \rho_0 \Delta k] \left(\frac{\hbar}{m_e}\right)^{3/2}}{|m|^{1/2} p_z \omega \omega_H^{5/2}}, \quad (36)$$

where $n_e = N/(\pi R^2 L)$ is the electron number density. The total cross-section is obtained by integrating over m :

$$\sigma_{\perp}^{\text{ff}} \equiv \int_{m_{\min}}^{m_{\max}} \sigma_{\perp}^{\text{ff}}(m) dm \simeq \frac{8Z'^2 \pi^3 \alpha_f^3 c^2 \hbar^2 n_e \exp(-2^{3/2} \rho_0 \Delta k)}{m_e p_z \omega \omega_H^2}, \quad \rho_0 \Delta k \gg 1. \quad (37)$$

In the integral, we have assumed $\bar{m} \approx m$ and $m_{\max} \gg m_{\min} = 1$.

In case (b) where both $\rho_0 \Delta k \ll 1$ and $\rho_{\bar{m}} \Delta k \ll 1$, from equations (29) and (25)

$$M_{\perp}^{\text{ff}} \simeq \frac{iZ' e^3}{\hbar L} \left(\frac{2\pi \hbar}{|m| \gamma \omega V_\gamma} \right)^{1/2}. \quad (38)$$

By again following the procedure which leads to equation (36) we now obtain

$$\sigma_{\perp}^{\text{ff}}(m) \xrightarrow{\rho_{\bar{m}} \Delta k \ll 1} \frac{16\pi^2 Z'^2 \alpha_f^3 \hbar^2 c^2 n_e}{|m| \omega \omega_H^2 p_z m_e}. \quad (39)$$

The total cross-section is given by

$$\sigma_{\perp}^{\text{ff}} = \int_{m_{\min}}^{m_{\max}} \sigma_{\perp}^{\text{ff}}(m) dm. \quad (40)$$

This integral contains the two limiting cases of $\rho_0 \Delta k \ll 1$ as m ranges from m_{\min} to m_{\max} : (i) A range of m where $\rho_{\bar{m}} \Delta k \ll 1$; (ii) a range where $\rho_{\bar{m}} \Delta k \gg 1$. Since $\rho_{\bar{m}} \Delta k \sim 1$ when $\bar{m} \approx m \simeq [2(\rho_0 \Delta k)^2]^{-1}$, equation (40) can be conveniently rewritten when $\rho_0 \Delta k \ll 1$ as

$$\sigma_{\perp}^{\text{ff}} = \int_{m_{\min}}^{1/[2(\rho_0 \Delta k)^2]} \sigma_{\perp}^{\text{ff}}(m) dm + \int_{1/[2(\rho_0 \Delta k)^2]}^{m_{\max}} \sigma_{\perp}^{\text{ff}}(m) dm, \quad (41)$$

where the first integral contains the case $\rho_{\bar{m}} \Delta k \ll 1$ and the second integral contains the case $\rho_{\bar{m}} \Delta k \gg 1$, and where the appropriate limiting form for the integrand is

$$\frac{16\pi^2 Z'^2 \alpha_f^3 \hbar^2 c^2 n_e}{p_z m_e \omega \omega_H^2} \ln \left[\frac{1}{2(\rho_0 \Delta k)^2 m_{\min}} \right]$$

after the $\sigma_{\perp}^{\text{ff}}(m)$ approximation for $\rho_{\bar{m}} \Delta k \ll 1$ of equation (39) is used. The second integral is

$$\frac{8\pi^3 Z'^2 \alpha_f^3 \hbar^2 c^2 n_e}{m_e p_z \omega \omega_H^2} \exp \left(-\frac{1}{2^{1/2} \rho_0^3 \Delta k^3} \right)$$

after the $\sigma_{\perp}^{\text{ff}}(m)$ approximation for $\rho_0 \Delta k \gg 1$ of equation (36) is used. Thus for $\rho_0 \Delta k \ll 1$, the total cross-section is approximately

$$\sigma_{\perp}^{\text{ff}} \simeq \frac{8\pi^3 Z'^2 \alpha_f^3 \hbar^2 c^2 n_e}{m_e p_z \omega_H^2} \left[\exp \left(-\frac{1}{2^{1/2} \rho_0^3 \Delta k^3} \right) - \frac{2 \ln (2 \rho_0^2 \Delta k^2)}{\pi} \right]. \quad (42)$$

When \mathbf{E} is parallel to \mathbf{H} , the cross-section for free-free absorption should be just the field-free result, since \mathbf{H} does not influence the motion of the electrons in this case. The matrix element for the absorption can be written

$$M_{\parallel}^{\text{ff}} = \frac{e A_0 \Delta k}{m_e c \omega} \langle 0, -|m|, k' | (V_{\bar{m}} - V_{\rho}) - V_{\bar{m}} | 0, -|m|, k \rangle \quad (43)$$

with

$$\hat{H}_{\text{int}} = \frac{e A_0 \hat{\pi}_3}{m_e c} e^{-i\omega t} \equiv \frac{e A_0}{m_e c} \frac{\partial}{\partial z} e^{-i\omega t}.$$

From equation (23) it then follows that

$$M_{\parallel}^{\text{ff}} = \frac{e A_0 \Delta k}{\omega m_e c} \langle k' | V_{\bar{m}} | k \rangle. \quad (44)$$

For a typical neutron star, $H \sim 5 \times 10^{12}$ gauss, $T \lesssim 10^8$ °K, so

$$\rho_0 \Delta k \sim 0.1 \ll 1. \quad (45)$$

In this case,

$$\sigma_{\parallel}^{\text{ff}} \xrightarrow{\rho_0 \Delta k \ll 1} \frac{8 Z'^2 \pi^3 \alpha_f^3 \hbar^2 c^2 n_e \exp(-2^{3/2} \rho_0 \Delta k)}{m_e p_z \omega^3} \quad (46)$$

which may be compared to the field-free result (Schwarzschild 1958)

$$\sigma_{\parallel}^{\text{ff}}(0) = \frac{16 Z'^2 \pi^3 \alpha_f^3 \hbar^2 c^2 n_e g_{\text{ff}}}{3^{3/2} m_e p_z \omega^3} \quad (47)$$

where g_{ff} is the Gaunt factor, of order unity.

The ratio of the cross-section for free-free absorption of photons with electric field polarization perpendicular and parallel to the magnetic field is

$$\frac{\sigma_{\perp}^{\text{ff}}(m)}{\sigma_{\parallel}^{\text{ff}}(m)} \equiv \left| \frac{M_{\perp}^{\text{ff}}}{M_{\parallel}^{\text{ff}}} \right|^2 = \frac{m_e^2 \omega^2}{\hbar^2 \Delta k^2} \left(\frac{|m|}{\gamma} \right) \left| \frac{\partial}{\partial \bar{m}} \ln \langle k' | V_{\bar{m}} | k \rangle \right|^2. \quad (48)$$

If we evaluate the matrix element of equation (44) for the various limiting cases of $\rho_0 \Delta k \gg 1$, $\rho_0 \Delta k \ll 1$, we obtain (Lodenquai 1972)

$$\frac{\sigma_{\perp}^{\text{ff}}(m)}{\sigma_{\parallel}^{\text{ff}}(m)} \simeq \frac{\omega^2}{\omega_H^2}, \quad \rho_0 \Delta k \gg 1; \quad (49)$$

$$\simeq (\omega/\omega_H)^2 \ln^{-2}(2), \quad \rho_0 \Delta k \ll 1. \quad (50)$$

Thus to a factor of order unity $\sigma_{\perp}^{\text{ff}} \sim (\omega/\omega_H)^2$ times the free-free cross-section in the absence of a magnetic field in both regimes. This same result also obtains from a completely classical calculation of these same processes.

V. BOUND-FREE TRANSITIONS

The properties of bound electrons in atoms in superstrong magnetic fields are quite different from the field-free case (Cohen, Lodenquai, and Ruderman 1970). For example, the ionization energy I of the outermost electron for an atom with atomic number $Z \sim 10$ –20 in a field $H = 2.2 \times 10^{12}$ gauss is very approximately given by $I = 160 \text{ eV} + 140 \ln Z$. The wave function of a bound electron in a given m state was approximated by (apart from normalization constants)

$$\psi = e^{im\phi} \xi^{|m|/2} e^{-z/2} f_m(z) \equiv |0, -|m|, k_i \rangle, \quad (51)$$

where $f_m(z) = (\alpha_m)^{1/2} \exp(-\alpha_m |z|)$ and α_m is a numerically determined variational parameter. Equation (51) assumes that the Coulomb field of the nucleus affects only the z -component of the electronic wave function in a superstrong magnetic field (Schiff and Snyder 1939). It is the transverse localization of the electron about the nucleus (situated at the origin) by the magnetic field that is responsible for the increased ionization energy. The

atoms in the superstrong magnetic field are cylindrical in shape with the axis of the cylinder along \mathbf{H} . If $H \sim 2 \times 10^{12}$ gauss, the ratio of the length to the radius of the hydrogen atom is about 10.

The Hamiltonian for bound-free transition is again given by

$$\hat{H} = \hat{H}_H - \frac{Z'e^2}{(z^2 + \rho^2)^{1/2}} + \hat{H}_{\text{int}}, \quad (52)$$

and the matrix element for bound-free transition

$$M = \int \psi_{k'} \hat{H}_{\text{int}} \psi_{k_i} dV, \quad (53)$$

where $\psi_{k_i}, \psi_{k'}$ are the initial and final wave functions, respectively. The final state $\psi_{k'}$ is a continuum wave function, but not a plane wave along z because of the Coulomb perturbation by the nucleus.

The perpendicular electric field matrix element for bound-free transition from the initial state $|0, -|m|, k_i\rangle$ to the final state $|0, -|m'|, k'\rangle$ is

$$\begin{aligned} M_{\perp}^{\text{bf}} &= \frac{i\omega e A_0}{c} \langle 0, -|m| + 1, k' | \rho \cos \phi | 0, -|m|, k_i \rangle \\ &= \frac{i\omega e A_0}{c} \langle 0, -|m| + 1 | \rho \cos \phi | 0, -|m| \rangle \langle k' | k_i \rangle \\ &= \frac{i\omega e A_0}{c} \left(\frac{|m|}{\gamma} \right)^{1/2} \langle k' | k_i \rangle, \end{aligned} \quad (54)$$

where use has been made of equations (17) and (20a). In Appendix B, an estimate of $\langle k' | k_i \rangle$ is shown to give

$$\langle k' | k_i \rangle \simeq -\frac{2Z'e^2}{\hbar\omega} \left(\frac{\alpha_m}{L} \right)^{1/2} \frac{\partial}{\partial m} K_0(|\alpha| \rho_m) \quad (55)$$

where L is a normalization length for the free electron in the magnetic field and $|\alpha| \equiv (k'^2 + \alpha_m^2)^{1/2}$. Under typical conditions of temperatures and magnetic field strengths in neutron-star atmospheres $k' \lesssim \alpha_m$ and $\rho_0 \alpha_m \ll 1$. We assume, therefore, that $|\alpha| \rho_m \ll 1$ where the maximum value of m is approximately Z , the atomic number of the nucleus. Then equation (29) applied to equation (55) gives

$$\langle k' | k_i \rangle \simeq \frac{Z'e^2}{\hbar\omega|m|} \left(\frac{\alpha_m}{L} \right)^{1/2}. \quad (56)$$

Therefore,

$$M_{\perp}^{\text{bf}} \simeq \frac{iZ'e^3 A_0}{\hbar c} \left(\frac{\alpha_m}{|m|\gamma L} \right)^{1/2}; \quad (57)$$

and the cross-section for the absorptive transition from a given initial m state is

$$\sigma_{\perp}^{\text{bf}}(m) = \frac{8\pi Z'^2 \alpha_f^3 \alpha_m \hbar c^2}{|m| \omega \omega_H p_z}. \quad (58)$$

The total cross-section is

$$\sigma_{\perp}^{\text{bf}} \simeq \int_{m_{\text{min}}}^{m_{\text{max}}} \sigma_{\perp}^{\text{bf}}(m) dm = \frac{8\pi Z'^2 \alpha_f^3 \hbar c^2 \{\alpha_m\} \ln Z}{\omega \omega_H p_z}, \quad (59)$$

where $\{\alpha_m\}$, the mean value of α_m , is given by

$$\{\alpha_m\} \ln Z \equiv \int_1^Z \frac{\alpha_m}{|m|} dm \quad (60)$$

(assuming $m_{\text{min}} = 1, m_{\text{max}} = Z$).

In the field-free case, $\sigma^{\text{bf}}(0)$ is approximately (Schwarzschild 1958)

$$\sigma^{\text{bf}}(0) = \frac{8\pi \alpha_f^5 Z'^4 m_e c^4 g_{\text{bf}}}{3^{3/2} \hbar \omega^3}, \quad (61)$$

where g_{bf} is the Gaunt factor for the bound-free transition. From equations (59) and (61) we have

$$\sigma_{\perp}^{\text{bf}}(H)/\sigma^{\text{bf}}(0) \simeq \omega^2/\omega_H\omega_H', \quad (62)$$

where

$$\omega_H' = \frac{(\alpha_f Z')^2 c^2 p_z m_e g_{\text{bf}}}{3^{3/2} \ln Z' \{\alpha_m\} \hbar^2}. \quad (63)$$

If $H \gtrsim 10^{12}$ gauss, we can use the results of Cohen *et al.* (1970) for the computed set of α_m to show that $\omega_H \approx \omega_H'$ (Lodenquai 1972). Then equation (62) is roughly equivalent to

$$\sigma_{\perp}^{\text{bf}}(H)/\sigma^{\text{bf}}(0) \approx (\omega/\omega_H)^2. \quad (64)$$

VI. BOUND-BOUND TRANSITION

The Thomson, free-free, and bound-free transitions are usually the three most important contributions in calculations of the opacity of stellar atmospheres. However, because of the huge magnetic fields and high temperatures existing in the atmospheres of neutron stars, it is not obvious that the bound-bound transitions do not make a significant contribution. An argument for a large bound-bound contribution is as follows: An atom with a thermal velocity v_{th} crossing a magnetic field H will experience an electric field ϵ (in its center-of-mass frame) given by

$$\epsilon = \frac{v_{\text{th}}}{c} \times H \quad (65)$$

with

$$v_{\text{th}} \sim (3kT/AM_p)^{1/2}, \quad (66)$$

where k is Boltzmann's constant, T the temperature, M_p the proton mass, and A the atomic weight of the nucleus. Then the maximum "induced" electric field is approximately

$$\epsilon_{\text{max}} \simeq (3kT/AM_p)^{1/2} H/c. \quad (67)$$

If $T \sim 10^7$ °K and $H \sim 5 \times 10^{12}$ gauss, then

$$\epsilon_{\text{max}} \simeq 2.5 \times 10^{12} A^{-1/2} \text{ volts cm}^{-1}. \quad (68)$$

For hydrogen, $A = 1$ and

$$\epsilon_{\text{max}}(H) \simeq 2.5 \times 10^{12} \text{ volts cm}^{-1}; \quad (69)$$

for iron, $A = 56$ and

$$\epsilon_{\text{max}}(\text{Fe}) \simeq 3 \times 10^{11} \text{ volts cm}^{-1}. \quad (70)$$

We shall estimate to what extent the shift in energy levels due to these very large and varying fields will appreciably broaden the spectral lines of the atoms in superstrong magnetic fields. If the energy difference between adjacent levels covers a sufficiently wide spectrum, then a wide spectrum of radiation could be absorbed, thus making a significant contribution to the opacity. We again assume the uniform H field to be along z . We can choose the vector potential

$$A \equiv A_y \hat{j} = (Hx + \Gamma) \hat{j}, \quad (71)$$

where Γ is an arbitrary constant, a choice which gives

$$(\nabla \times A)_z = H, \quad \nabla \cdot A = 0. \quad (72)$$

The total Hamiltonian for the electron in this gauge is

$$\begin{aligned} \hat{H} &= \frac{1}{2m_e} \left[p_y - \frac{e}{c} (Hx + \Gamma) \right]^2 + \frac{p_x^2 + p_z^2}{2m_e} - e\epsilon x - \frac{Ze^2}{r} \\ &= \frac{p^2}{2m_e} - \frac{e}{m_e c} (Hx + \Gamma) \hat{p}_y - e\epsilon x - \frac{Ze^2}{r} + \frac{e^2}{2m_e c^2} (Hx + \Gamma)^2 \\ &= \frac{\hat{p}^2}{2m_e} - \omega_H x \hat{p}_y - \frac{e\Gamma}{m_e c} \hat{p}_y + \frac{1}{2} m_e \omega_H^2 x^2 + \frac{e^2 H \Gamma x}{m_e c^2} + \frac{e^2 \Gamma^2}{2m_e c^2} - e\epsilon x - \frac{Ze^2}{r}. \end{aligned} \quad (73)$$

The electric field ϵ , given in equation (65), ranges from zero, when v_{th} is parallel to H , to $v_{th}H/c$ when v_{th} is transverse to H . We have defined \hat{p} by

$$\hat{p}^2 = \hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2.$$

Since Γ is an arbitrary constant, we can choose it such that $e^2 H \Gamma x m_e c^2 = e \epsilon x$, i.e.,

$$\Gamma = m_e c^2 \epsilon / H e. \quad (74)$$

Then the Hamiltonian reduces to

$$\hat{H} = \frac{\hat{p}^2}{2m_e} - \omega_H x \hat{p}_y - \frac{e\Gamma}{m_e c} \hat{p}_y + \frac{1}{2} m_e \omega_H^2 x^2 + \frac{e^2 \Gamma^2}{2m_e c^2} - \frac{Ze^2}{r} = \hat{H}_H - \frac{e\Gamma}{m_e c} \hat{p}_y + \frac{e^2 \Gamma^2}{2m_e c^2} - \frac{Ze^2}{r}, \quad (75)$$

where

$$\hat{H}_H = \frac{\hat{p}^2}{2m_e} - \omega_H x \hat{p}_y + \frac{1}{2} m_e \omega_H^2 x^2$$

is just the Hamiltonian of an otherwise free electron in an external magnetic field, with the vector potential

$$A \equiv A_y \hat{j} = H x \hat{j}.$$

We assume known the exact solution of the Hamiltonian

$$\hat{H}_H - \frac{Ze^2}{r} + \frac{e^2 \Gamma^2}{2m_e c^2}, \quad (76)$$

and treat $e\Gamma \hat{p}_y / m_e c$ as a perturbation. The solution to equation (76) is essentially that for an electron in the presence of the Coulomb field of the nucleus and a uniform external magnetic field, which gave rise to the ‘‘cylindrical’’ atoms that were treated by Cohen *et al.* (1970). The only difference is the constant $e^2 \Gamma^2 / 2m_e c^2$ which introduces the same shift to all the energy levels. We have taken the perturbation to be $(e\Gamma / m_e c) \hat{p}_y$, with a maximum of

$$\hat{H}_{\max}^{(1)} = (e\Gamma / m_e c) \hat{p}_y \equiv v_{th} \hat{p}_y. \quad (77)$$

To second order, the maximum shift of the m th energy level is

$$\Delta E_m^{(2)} = v_{th}^2 \sum_I \frac{\langle m | \hat{p}_y | I \rangle \langle I | \hat{p}_y | m \rangle}{E_I - E_m}, \quad (78)$$

where I refers to the intermediate states. (We note that, because of symmetry of the ‘‘unperturbed’’ solution, $\langle m | \hat{p}_y | m \rangle$ is zero.) For the ground state, we can bound $\Delta E_0^{(2)}$ by

$$\Delta E_0^{(2)} = v_{th}^2 \sum_I \frac{|\langle 0 | \hat{p}_y | I \rangle|^2}{E_I - E_0} \leq v_{th}^2 \frac{\langle 0 | \hat{p}_y^2 | 0 \rangle}{E_I - E_0} \quad (79)$$

with $\langle 0 | \hat{p}_y^2 | 0 \rangle \simeq \frac{1}{2} m_e \hbar \omega_H$. For iron at $T \sim 10^7$ K and $H \sim 5 \times 10^{12}$ gauss, $v_{th} \simeq 10^7$ cm s $^{-1}$, and $E_1 - E_0 \simeq 10^2$ eV. Then $\Delta E_0 \simeq 3$ eV. The maximum relative shift between the $m = 0$ and $m = 1$ levels, i.e., $|\Delta E_0 - \Delta E_1|$, should be of this order or as will be shown below even smaller. (The minimum net shift due to ϵ is of course zero, corresponding to v_{th} parallel to H .)

We consider now the shifts between adjacent levels for levels with large m . We have for the net maximum difference between adjacent energy levels from equation (78)

$$\Delta E_m^{(2)} - \Delta E_{m-1}^{(2)} = v_{th}^2 \sum_I \left[\frac{|\langle m | \hat{p}_y | I \rangle|^2}{E_I^{(0)} - E_m^{(0)}} - \frac{|\langle m-1 | \hat{p}_y | I \rangle|^2}{E_I^{(0)} - E_{m-1}^{(0)}} \right]. \quad (80)$$

The leading terms in $\Delta E_m^{(2)}$, $\Delta E_{m-1}^{(2)}$ are contributed by the matrix elements with adjacent levels. For these leading terms, equation (80) reduces to

$$\begin{aligned} \Delta E_m^{(2)} - \Delta E_{m-1}^{(2)} \simeq v_{th}^2 & \left[\left(\frac{|\langle m | \hat{p}_y | m+1 \rangle|^2}{E_{m+1}^{(0)} - E_m^{(0)}} - \frac{|\langle m | \hat{p}_y | m-1 \rangle|^2}{E_m^{(0)} - E_{m-1}^{(0)}} \right) \right. \\ & \left. - \left(\frac{|\langle m-1 | \hat{p}_y | m \rangle|^2}{E_m^{(0)} - E_{m-1}^{(0)}} - \frac{|\langle m-1 | \hat{p}_y | m-2 \rangle|^2}{E_{m-1}^{(0)} - E_{m-2}^{(0)}} \right) \right]. \end{aligned} \quad (81)$$

In the superstrong field limit, a generalization of the formula of Haines and Roberts (1969) for the energy of the m th level (without screening) is

$$E_m^{(0)} \simeq Z^2 E_{\text{Ry}} \ln^2 \left(\frac{\alpha_0}{m^{1/2} Z \rho_0} \right). \quad (82)$$

For large m , the maximum separation between adjacent m levels is then

$$\Delta E_m^{(2)} \equiv E_m^{(0)} - E_{m-1}^{(0)} \simeq \frac{\partial E_m^{(0)}}{\partial m} \simeq \frac{Z^2 E_{\text{Ry}}}{m} \ln \left(\frac{\alpha_0}{m^{1/2} Z \rho_0} \right). \quad (83)$$

We use this approximation in the denominator of equation (81) and approximate

$$|\langle m | \hat{p}_y | m-1 \rangle|^2 \lesssim |\langle m | \hat{p}_y | m \rangle|^2 \simeq \frac{1}{2} m_e \hbar \omega_H. \quad (84)$$

Then from equation (83) we have the approximate bound to the m dependence:

$$\Delta E_m^{(0)} \sim m^{-1} \ln m.$$

Then the leading m dependence of equation (81) is at most given by

$$|\Delta E_m^{(2)} - \Delta E_{m-1}^{(2)}| \propto \left[\frac{\partial}{\partial m} \left(\frac{m}{\ln m} \right) - \frac{\partial}{\partial m} \left(\frac{m-1}{\ln(m-1)} \right) \right] \simeq \frac{\partial^2}{\partial m^2} \left[\frac{m}{\ln m} \right] \propto [m(\ln m)^2]^{-1}, \quad (85)$$

and we see that the net shift between adjacent levels for large m decreases at least as fast as $[m(\ln m)^2]^{-1}$. Since the contributions from the lowest levels were shown to be small, the contributions from the large m levels should be even smaller.

Relative to $\epsilon \rho_m \sim 10^2 Z^{1/2}$ eV, the potential difference across an outer atomic orbital, there is only a very small shift between adjacent levels of our “cylindrical” atoms. We note that if the atom consisted of just two levels, we would get the expected large shift in the presence of the ϵ field. However, in fact, there is an infinite number of levels. A given level tends to be shifted away from its adjacent levels by the ϵ field. Since there are adjacent levels above and below the level under consideration, the shifting tendencies are in opposite directions, and quite effectively cancel out each other in this case. This strong-magnetic-field case is mathematically quite similar to the problem of a charged simple harmonic oscillator in an external electric field. The Hamiltonian in that case is

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m \omega^2 x^2 - Fx = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m \omega^2 (x - x_0)^2 + \text{const.},$$

where $x_0 \equiv F/m\omega^2 = \text{constant}$. The Hamiltonian has the pure oscillator form, but with a shifted equilibrium position. However, the difference between energy levels is still $\hbar\omega$ since all the levels are shifted by the same constant amount.

If we were to treat hydrogen atoms instead of large- A atoms as we did above, v_{th} would be greater and $\Delta E_m^{(0)}$ would be small, each tending to increase the fractional shift between adjacent levels. So for hydrogen we might expect a large relative shift in the energy levels under the conditions existing in neutron star atmospheres. Such a shift in energy levels can be so large as to cause the hydrogen atoms to be ionized.

APPENDIX A

DERIVATION OF EQUATION (20)

Equation (20a) can be obtained as follows. We have

$$\begin{aligned} \langle 0, -|m| + 1, k' | \rho \cos \phi | n_\rho, -|m|, k'' \rangle \\ \equiv \langle k' | k'' \rangle \left(\frac{C_{n_\rho, -|m|} C_{0, -|m|+1}}{\gamma} \right)^{1/2} \int_0^\infty e^{-\xi} \xi^{|m|-1/2} \xi^{|m|/2} F(-n_\rho, |m| + 1, \xi) \xi^{1/2} d\xi \\ = \delta_{k'k''} \left(\frac{C_{n_\rho, -|m|} C_{0, -|m|+1}}{\gamma} \right)^{1/2} \int_0^\infty e^{-\xi} \xi^{|m|} F(-n_\rho, |m| + 1, \xi) d\xi. \end{aligned} \quad (A1)$$

Now

$$\int_0^\infty e^{-\xi} \xi^{|m|} F(-n_\rho, |m| + 1, \xi) d\xi \equiv J_{-n_\rho, |m|+1}^{|m|} = \frac{(-)^{n_\rho} \Gamma(|m| + 1) (\lambda - 1)^{n_\rho}}{(|m| + 1)(|m| + 2) \cdots (|m| + n_\rho - 1)} \frac{d^{n_\rho} (\lambda^{-|m|-1})_{\lambda=1}}{d\lambda^{n_\rho}} \quad (A2)$$

(Landau and Lifshitz 1965). This integral is zero unless $n_\rho = 0$ in which case we get

$$J^{|m|}_{0, |m|+1} = |m|! . \quad (\text{A3})$$

Therefore

$$\langle 0, -|m| + 1, k' | \rho \cos \phi | n_\rho, -|m|, k'' \rangle = \delta_{k'k''} \delta_{n_\rho, 0} (|m|/\gamma)^{1/2}, \quad (\text{A4})$$

where we have put in the values of the normalization constants.

Similarly, to obtain equation (20b) we have

$$\langle n_\rho, -|m| + 1, k'' | \rho \cos \phi | 0, -|m|, k \rangle = \langle k'' | k \rangle \left(\frac{C_{n_\rho, -|m|+1} C_{0, -|m|}}{\gamma} \right)^{1/2} \int_0^\infty e^{-\xi} \xi^{|m|} F(-n_\rho, |m|, \xi) d\xi. \quad (\text{A5})$$

Now

$$\begin{aligned} \int_0^\infty e^{-\xi} \xi^{|m|} F(-n_\rho, |m|, \xi) d\xi &= J^{|m|}_{-n_\rho, |m|} = |m|, & n_\rho &= 0, \\ &= -(|m| - 1)!, & n_\rho &= 1, \\ &= 0, & \text{otherwise,} \end{aligned} \quad (\text{A6})$$

where we have used equation (A2).

APPENDIX B

DERIVATION OF EQUATION (55)

We consider the matrix element

$$\langle k' | k_i \rangle \equiv \int_{-\infty}^{\infty} g_{m'}^*(z) f_m(z) dz \quad (\text{B1})$$

where $g_{m'}(z)$ is the z -component of the continuum wave function, with angular momentum m' . With the approximation of Schiff and Snyder (1939) we have for the Schrödinger equations for $f_m(z)$ and $g_{m'}^*(z)$:

$$\frac{-\hbar^2}{2m_e} \frac{d^2 f_m(z)}{dz^2} + v_i(z) f_m(z) = -|E_B| f_m(z), \quad (\text{B2})$$

$$\frac{-\hbar^2}{2m_e} \frac{d^2 g_{m'}^*(z)}{dz^2} + v_f(z) g_{m'}^*(z) = E_{k'} g_{m'}^*(z), \quad (\text{B3})$$

where E_B is the binding energy of the bound electron. If we multiply equation (B2) by $g_{m'}^*(z)$ and equation (B3) by $f_m(z)$, subtract the two, and then integrate over z , we get

$$\begin{aligned} \frac{-\hbar^2}{2m_e} \int_{-\infty}^{\infty} \left[f_m(z) \frac{d^2 g_{m'}^*(z)}{dz^2} - g_{m'}^*(z) \frac{d^2 f_m(z)}{dz^2} \right] dz + \int_{-\infty}^{\infty} \left[v_f g_{m'}^*(z) f_m(z) - v_i f_m(z) g_{m'}^*(z) \right] dz \\ = \int_{-\infty}^{\infty} [E_{k'} f_m(z) g_{m'}^*(z) + |E_B| f_m(z) g_{m'}^*(z)] dz; \end{aligned} \quad (\text{B4})$$

i.e.,

$$\frac{-\hbar^2}{2m_e} \int_{-\infty}^{\infty} [f_m(z) \nabla_z^2 g_{m'}^*(z) - g_{m'}^*(z) \nabla_z^2 f_m(z)] dz + \int_{-\infty}^{\infty} (v_f - v_i) g_{m'}^*(z) f_m(z) dz = (E_{k'} + |E_B|) \int_{-\infty}^{\infty} g_{m'}^*(z) f_m(z) dz. \quad (\text{B5})$$

Now

$$[f_m(z) \nabla_z^2 g_{m'}^*(z) - g_{m'}^*(z) \nabla_z^2 f_m(z)] = \nabla_z \cdot [f_m(z) \nabla_z g_{m'}^*(z) - g_{m'}^*(z) \nabla_z f_m(z)]. \quad (\text{B6})$$

So

$$\int_{-\infty}^{\infty} [f_m(z) \nabla_z^2 g_{m'}^*(z) - g_{m'}^*(z) \nabla_z^2 f_m(z)] dz = 0$$

in equation (B5) since $f_m(\pm\infty) = g_{m'}(\pm\infty) = 0$. Equation (B5) then reduces to

$$\int_{-\infty}^{\infty} g_{m'}^*(z) f_m(z) dz = \frac{1}{\hbar\omega} \int_{-\infty}^{\infty} (v_f - v_i) g_{m'}^*(z) f_m(z) dz, \quad (\text{B7})$$

since for photoelectric absorption, $|E_B| + E_{k'} = \hbar\omega$. On the right-hand-side of equation (B7) we can now take

$g_m(z)$ to be a plane wave, and $f_m^*(z) = f_m(z) = \exp(-\alpha_m|z|)$ even though they are not orthogonal and cannot be used directly in evaluating the left-hand-side of equation (B7). Then

$$\langle k' | k_i \rangle = \int_{-\infty}^{\infty} g_m^*(z) f_m(z) dz \simeq \frac{1}{\hbar\omega} \left(\frac{\alpha_m}{L} \right)^{1/2} \int_{-\infty}^{\infty} (v_f - v_i) \exp(-ik'z - \alpha_m|z|) dz. \quad (\text{B8})$$

Now

$$v_i = -\frac{Z'e^2}{(z^2 + \rho_m^2)^{1/2}}; \quad v_f = -\frac{Z'e^2}{(z^2 + \rho_{m'}^2)^{1/2}},$$

where

$$m = -|m|, \quad m' = -|m| + 1, \quad \rho_m \simeq (2|m|)^{1/2} \rho_0,$$

and therefore

$$v_f - v_i \simeq -Z'e^2 \frac{\partial}{\partial m} \frac{1}{(z^2 + \rho_m^2)^{1/2}}. \quad (\text{B9})$$

Therefore equation (B8) becomes

$$\langle k' | k_i \rangle \simeq -\frac{Z'e^2}{\hbar\omega} \left(\frac{\alpha_m}{L} \right)^{1/2} \frac{\partial}{\partial m} \int_{-\infty}^{\infty} \frac{\exp(-ik'z - \alpha_m|z|)}{(z^2 + \rho_m^2)^{1/2}} dz = -\frac{2Z'e^2}{\hbar\omega} \left(\frac{\alpha_m}{L} \right)^{1/2} \frac{\partial}{\partial m} K_0(|\alpha|\rho_m) \quad (\text{B10})$$

when we have used equation (27). In the above we have defined

$$|\alpha| \equiv (k'^2 + \alpha_m^2)^{1/2}. \quad (\text{B11})$$

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